### **1,10-Phenanthroline** 66-71-7 | DTXSID1025857

## **Model Performance**

Model	Data	
Model	Dala	

# Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

#### Model Results

Predicted value: 4.58

Global applicability domain: Inside

Local applicability domain index: 4.67e-01

Confidence level: 6.90e-01

## Nearest Neighbors from the Training Set

Image not found

4-Isobutylmorpholine

Measured: 1.78 Predicted: 2.69

Image not found

6-Nitrobenzimidazole

Measured: 2.51 Predicted: 3.81

Image not found

Triethylamine

Measured: 4.90 Predicted: 5.95

Image not found

Molinate

Measured: 25.7 Predicted: 14.8

Image not found

Piperidine, 1-methyl-Measured: 4.47 Predicted: 5.88